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Effect of Topological Disorder on Transport

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Abstract

We have studied the combined effect of topological and substitutional impurities on the band structure of solids. An interplay of the two types of impurities can make the band asymmetric around the band center and changes it non trivially.
Key words: Topological defect, Fano resonance, Conductance.

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There have been several recent studies on substitutional impurities and their effect on transport properties of solids[1,2]. Whereas the study of intrinsic topological disorder associated with randomness in geometries has recently attracted the attention of many. Some such materials are percolation clusters, fractals and branched polymers. More recently there is an entire new branch of systems called mesoscopic systems[3,4] in which the classical transport mechanisms do not hold. Transport in them is studied by quantum mechanics and the geometry of the system determines the transport properties. It may also explain the transport properties of dirty quantum wires. Conductance of such systems is related to the quantum mechanical transmittance by Landauers two probe conductance formula[5].

Transport properties across such a geometrical structure was studied by Guinea and Verges[6] in the tight binding model where all their sites are perfect. The structure is now more popularly known as T shaped structure. There is a main wire that extends from $-\infty$ to ∞ and there is a finite side chain attached to it fig. (1). The system is chosen to be 1-D and it represents the real situation of such quantum wires and quasi 1-D systems at low temperatures when the Fermi energy is so adjusted that only the first subband propagates[7]. Such 2-D systems have also been studied in the Tight Binding(TB) and continuum model and such structures have been proposed as ballistic transistors and switches[8].

In this paper we have studied the effect of topological defect on the transport properties of 1-D and quasi 1-D solids. The tight binding model is more appropriate for describing solids, where the electrons feel the periodicity of the underlying lattice and has a band structure due to it. We consider a realistic situation by incorporating substitutional impurities along with the geometrical impurity and study the interplay between the two in modifying the band structure of the solid. A real system will in general have more than one such geometrical defects with substitutional impurities in it, aswellas in the main chain. In this article we show that if the substitutional impurity is located inside the topological defect then only one such defect (single impurity problem) changes the band and hence the transport properties of the solid non trivially. We have considered an infinite chain of perfect sites with a geometrical defect made up of a few sites and attached to the infinite chain (fig. (1)). There are some substitutional impurities in this finite chain. A detailed study of the real situation will be presented later.

When the side chain consists of a single site as in fig. 1 the impurity can lie at either B, or C or at both the sites. The perfect sites are taken to be of zero site energy according to usual practice and the hopping parameter V is taken one everywhere. The site energies at B and C are ϵ_B and ϵ_C respectively. We solve this problem analytically using the same procedure as in [6]. That is the effects of the sites C and B can be replaced by an energy dependent self energy acting only on the site B i.e., $\Sigma_B(E)$. So we have a single impurity in an infinite chain whose effective site energy is $\Sigma_B(E)$.

Using standard Greens function technique we find

$$\Sigma_B(E) = \frac{V^2}{(E - \epsilon_C)} + \epsilon_B \tag{1}$$

If we put ϵ_B=0 (ϵ_C=0) then we get the results for the impurity being at the site C (B). Putting both zero we get the same result as that of ref[6]. In fig. (2) we have plotted the transmission coefficient versus energy for a case $\epsilon_B = \epsilon_C = 0$. This case exhibits a symmetric band. Using the standard tight binding techniques[6] we have calculated the transmission across the sample for two cases ($\epsilon_B \neq 0$, $\epsilon_C = 0$;$\epsilon_B = 0$, $\epsilon_C \neq 0$). They are shown in figs (3) and (4). We observe strong energy dependence of the transport properties with the conductance vanishing at certain energies, as in Guinne Vergies. But the new observation is that the *pass band becomes completely asymmetric* in fig. (3) and (4) *with a definite line shape*. In the presence of either substitutional impurities or geometric defects, the Tight Binding Hamiltonian has particle hole symmetry and as a result the distribution of its eigenenergies, transmission coefficient etc. are all symmetric around E=0[6]. Because of the particle hole symmetry of the Hamiltonian, the particle band and the hole band differ by only an overall sign apart from some unimportant additive constants, that can always be set to zero. The negative sign in front of the hole band can be removed by a transformation k$\rightarrow$k+π/a where a is a lattice constant. So with the help of this (half a band) translation (which is just a shift of origin) the hole band can be made to coincide with the particle band completely. The asymmetric band in our case suggests that the particle hole symmetry is lost. It happens because of the special form of the effective self energy $\Sigma_B(E)(\neq \Sigma_B(-E))$ which arises solely due to an interplay of geometrical and substitutional impurity. We know that transmission zeros are exhibited by only geometric scatterers[6,11] but as seen in fig (4) the position of the zero is determined by the strength of ϵ_c. Throughout the sample we have set hopping term V$\equiv$1.

We now consider a situation wherein side chain is composed of several lattice points or atoms. Transport across such a long side chain is studied numerically using the vector recursion procedure [9]. We slightly alter the algorithm to tackle such geometries. First we choose all sites in the side chain to be perfect(ϵ = 0) and take the site at the junction to be of energy ϵ_J. This is the discrete version of the work of Tekman and Bagwell[10]. The side chain behaves as a resonant cavity that sustains standing waves. There are also the continuum states in the main chain. So an incident electron has two alternate paths. One is without entering the side chain and the other is the electron enters the side chain, spends some extra time and then comes out to mix with the continuum. The total transmission is dictated by interference between these two alternating paths. The defect site at the junction causes a weak coupling of the states in the resonant cavity with the continuum states in the main chain. In such a situation the resonances in the Tight Binding Model band are not the usual Breit Wigner resonances (that are symmetric about the poles of complex transmission amplitude) but the asymmetric Fano resonances (that are asymmetric about the poles of the complex transmission amplitude) [11]. The new observation in the discrete model that we have considered is that these asymmetric resonances make the entire pass band of the Tight Binding Model asymmetric about E=0. The distribution of the poles and zeros over the entire band is asymmetric about E=0. In fig. (5) we have ploted transmittance versus energy of such a system with 20 sites in the side chain. We have plotted for three values of ϵ_J=0 (dotted curve), -1 (dashed curve) and -2 (solid curve). Note that when ϵ_J=0 we get a perfect system as that considered in[6]. The vector recursion technique also allows us to incorporate substitutional impurities in the side chain. Note that the resonances at the band edges when ϵ_J=0 are asymmetric because the states at the band edges are more localized than that at the band center. But the band is still symmetric about the band center. But for non zero ϵ_J all the resonances inside the band become Fano resonances and the symmetry of band is destroyed. Such a long chain will exhibit many zeros within a given energy range (the pass band). As the length is gradually made shorter the zeros start moving out towards the band edges and goes out of the pass band. The shortest case is that of fig. (1) where a single zero is left in the pass band and the asymmetry is still maintained as in fig. (3). Hence the line shape of the Fano resonances determine the line shape of the transmission band. This may help to engineer the line shape of the transmission band of 1-D and quasi-1-D systems by tuning the strength of a defect site inside an artificially built geometric structure.

Next we choose the site energies in the side chain randomly between -W/V and +W/V. The side chain consists of 20 sites. Again we see that the fano resonances in the band makes the band asymmetric. The origin of Fano resonances in this case is however slightly different from that of the case discussed by Bagwell. Here the disordered side chain causes the Anderson localization of the states in it. Such localized states are weakly coupled to the continuum states of the main chain and give rise to the Fano type resonances. In fig. (6) we plot transmittance versus energy for such a chain for three values of $W/V=0$ (dotted line), 1 (dashed line) and 2 (solid line). Again $W/V=0$ is the case of perfect sites considered in[6]. When this chain is gradually made shorter then again the zeros move out of the band and in the shortest situation we have the case of fig(1) with a substitutional impurity at C which gives the asymmetric band as in fig(4).

We conclude by stating the main results of this work. A single substitutional impurity situated in a geometrical defect can drastically modify the band of the host solid and alter its transport properties. Such an interplay of geometrical and substitutional impurity can make the band of the host solid asymmetrical, signifying the breakdown of particle hole symmetry. The form of the self energy signifies that one or a few such defects will change the band nontrivially in quasi 1-D or 2-D.

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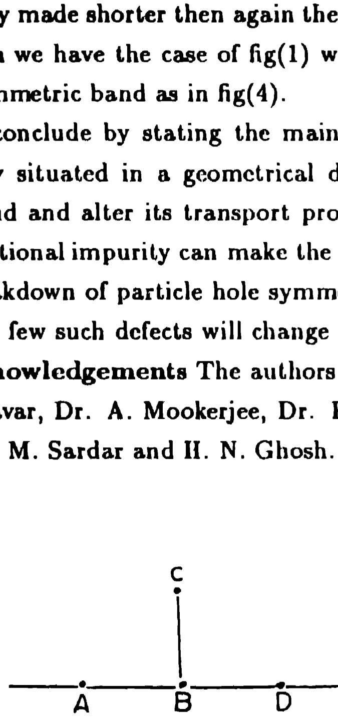

fig.1 A finite side chain attached to an infinite wire.

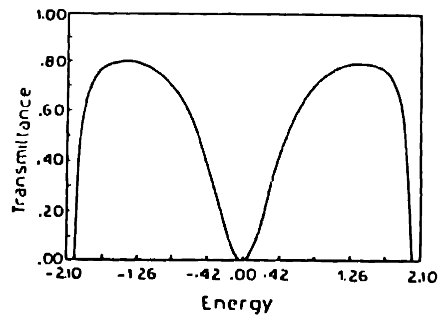

fig.2 Transmittance vs energy when all sites are perfect.

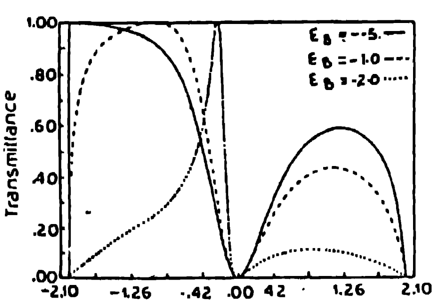

fig.3 Transmittance vs energy when a single substitutional impurity is at B.

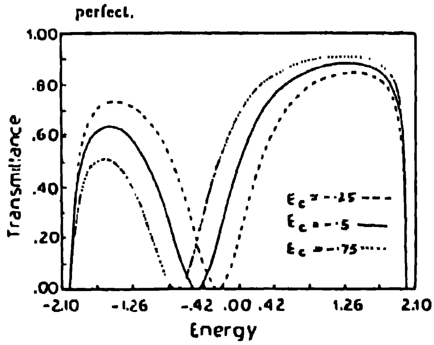

fig.4 Transmittance vs energy when a single substitutional impurity is at C.

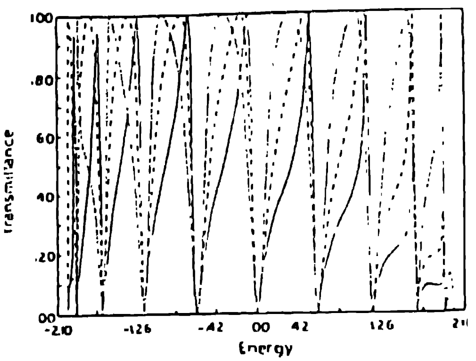

fig.5 Transmittance vs energy across a long finite side chain with a single impurity at the junction.

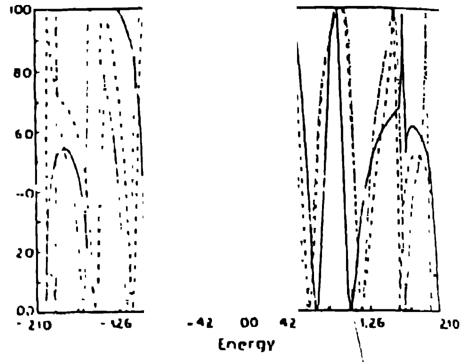

fig.6 Transmittance vs energy across a long finite disordered side chain.

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